ROTATIONAL SPECTROSCOPY OF THE METHYL GLYCIDATE-WATER COMPLEX

JASON GALL, JAVIX THOMAS, ZHIBO WANG, WOLFGANG JAEGER, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*.

Many biologically important molecules are chiral and perform their biological functions in an aqueous medium. In this study, we investigate the intermolecular interactions of methyl glycidate, a chiral epoxy ester, with water using rotational spectroscopy. We examine the competition among the three hydrogen-bond acceptor sites at methyl glycidate: the epoxy oxygen, the carbonyl oxygen, and the ester oxygen when interacting with water. We also probe how interaction with water modifies the methyl internal rotation barriers and conformational distribution of methyl glycidate. The possible large amplitude and tunnelling motions associated with water are investigated and analyzed.